RECONSTRUCTION OF TERM DIAGRAMS WITHOUT USING A MODEL HAMILTONIAN

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The fundamental Ritz combination principle [1] originally found for atoms has also been applied to molecules as a method to reconstruct the energy states from measured lines without relying on any model Hamiltonian. In 2006 Nesbitt and coworkers [2] proposed to apply it to protonated methane, CH_5^+, which was first done in 2015 [3] and extended in 2017 [4] by our group. Currently, we are elaborating this method to a universal, easy to use tool which can be used for arbitrary spectra. Essentials of the program and examples, including the floppy He-H_3^+ system, will be discussed.

[1] W. Ritz, On a new law of series spectra, Astrophys. J. 28 (1908), p. 237.
[2] C. Savage, F. Dong, D.J. Nesbitt, Toward a quantum-mechanical understanding of the high-resolution infrared spectrum of CH_5^+, in: Contribution TA05, 61st International Symposium on Molecular Spectroscopy, Columbus, OH, USA, 2006.
[3] Oskar Asvany, Koichi M. T. Yamada, Sandra Brünken, Alexey Potapov, Stephan Schlemmer. Experimental ground-state combination differences of CH_5^+. Science, 347 (2015), pp. 1346-1349.
[4] S. Brackertz, S. Schlemmer, O. Asvany, Searching for new symmetry species of CH_5^+ – From lines to states without a model, J. Mol. Spectrosc. 342 (2017), p. 73-82.